Variational and Geometric Aspects of Compatible Discretizations

May 12, 2004

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Supported in part by

MICS
Mathematical, Information, and Computational Sciences

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Why are we here?

We conclude…that exterior calculus is here to stay, that it will gradually replace tensor methods in numerous situations where it is the more natural tool, that it will find more and more applications because of its inner simplicity. Physicists are beginning to realize its usefulness; perhaps it will soon make its way into engineering.

H. Flanders,

There's generally a time lag of some fifty years between mathematical theories and their applications…

1950 + 50 = 2000

It's about time !

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Acknowledgments and Sources

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  - R. Kotiuga, PhD Thesis, (1984), PIERS32 (2001)
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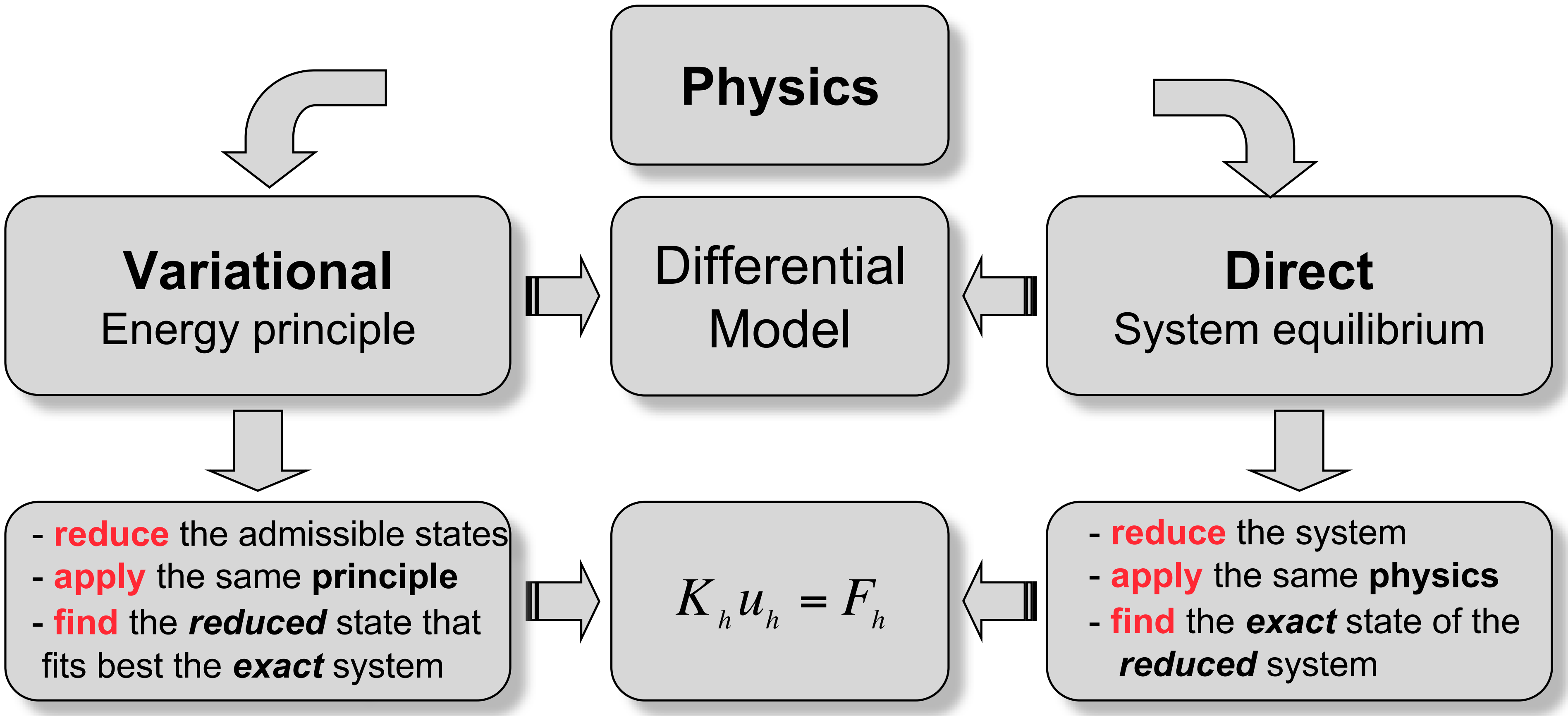
  - C. Mattiussi, JCP (1997)
  - L. Demkowicz, TICAM99-06, (1999)
  - R. Hiptmair, Numer. Math., 90 (2001), PIERS32
  - D. Arnold, ICM, Beijing, (2002)

- **Thanks to**
  - D. Arnold (IMA)
  - M. Gunzburger (FSU)
  - R. Lehoucq (SNL)
  - R. Nicolaides (CMU)
  - A. Robinson (SNL)
  - M. Shashkov (LANL)
  - C. Scovel (LANL)
  - K. Trapp (CMU)

How different people discretize



Discretization is a model reduction that replaces a physical process by a parametrized family of algebraic equations.

What do we want to know?

1. **Is the sequence of algebraic equations well-behaved?**
   - are all problems **uniquely and stably** (in *h*) solvable?
   - do solutions **converge** to the exact solutions as $h \rightarrow 0$?

2. **Are physical and discrete models compatible?**
   - are solutions **physically** meaningful
   - do they **mimic**, e.g., invariants, symmetries of actual states

3. **How to make a compatible & accurate discretization?**
   - how to **choose** the variables and where to place them;
   - how to avoid **spurious** solutions.

We revisit earlier discussion with a particular focus on how

- **variational** compatibility (Arnold)
- **geometric** compatibility (Nicolaides, Shashkov)

can be used to answer these questions.

A sequence of linear systems vs. a single linear system

$Ku = F$

$K_h u_h = F_h$

Solvability

$Ku = 0 \Rightarrow u \equiv 0$

$K_h u_h = 0 \Rightarrow u_h \equiv 0$

Stability

$$\frac{\|\Delta u\|}{\|u\|} \le \|K\| \|K^{-1}\| \frac{\|\Delta F\|}{\|F\|}$$

$$\frac{\|\Delta u_h\|}{\|u_h\|} \le \|K_h\| \|K_h^{-1}\| \frac{\|\Delta F_h\|}{\|F_h\|}$$

Stability of linear systems arising from PDEs cannot be assessed by standard condition number:

$$\|K\| \|K^{-1}\| = \frac{\lambda_{\max}}{\lambda_{\min}} \Rightarrow O(h^{-2})$$

$$\left.\begin{aligned} \|u_h\|_X^2 &= u_h^T S_h u_h \\ \|K_h\| &= \sup_{v_h} \frac{\|K_h v_h\|_*}{\|v_h\|_X} \end{aligned}\right\}$$

$$(\mathbf{R}^n, \|\cdot\|_X) \underset{K_h^{-1}}{\overset{K_h}{\rightleftarrows}} (\mathbf{R}^n, \|\cdot\|_*)$$

$$\left\{\begin{aligned} \|u_h\|_* &= \sup_{v_h} \frac{v_h^t u_h}{\|v_h\|_X} \\ \|K_h^{-1}\| &= \sup_{v_h} \frac{\|K_h^{-1} v_h\|_X}{\|v_h\|_*} \end{aligned}\right.$$

$$\|K\| \|K^{-1}\| \le ???$$

Stability of a sequence

$$\|K_h\| \le \alpha \quad \& \quad \|K_h^{-1}\| \le \frac{1}{\mathrm{glb}(K_h)} \quad \Rightarrow \quad \|K_h\|\|K_h^{-1}\| \le \frac{\alpha}{\mathrm{glb}(K_h)}$$

glb suggested by G. **Golub**

$$\mathrm{glb}(K_h) = \inf_{u_h} \frac{\|K_h u_h\|_*}{\|u_h\|_X} = \inf_{u_h} \sup_{v_h} \frac{v_h^T K_h u_h}{\|v_h\|_X \|u_h\|_X}$$

$$\inf_{u_h} \sup_{v_h} \frac{v_h^T K_h u_h}{\|v_h\|_X \|u_h\|_X} \ge \gamma > 0 \quad \Rightarrow \quad \|K_h\|\|K_h^{-1}\| \le \frac{\alpha}{\gamma}$$

stability = α and γ are independent of h

$$\underbrace{\min_{u_h} \max_{v_h} \frac{v_h^T K_h u_h}{\left(v_h^T S_h v_h\right)^{1/2} \left(u_h^T S_h u_h\right)^{1/2}}}_{\sigma_1(K_h, S_h)} \ge \gamma$$

The smallest generalized singular value of K_h must be bounded away from zero, **independent of** ***h*****.**

Variational Methods

Galerkin approximation of operator equations

$$D(A) \subset X \qquad\qquad D(A) \supset X_h$$

$$\begin{array}{cccc} & X & Au = f & f \\ P_h & \downarrow & & \downarrow\ Q_h \\ & X_h & Q_h A u_h = f_h & f_h \end{array}$$

$$f \in R(A) \subset Y \qquad\qquad f_h \in Y_h \not\subset R(A)$$

Galerkin theorem

solvability

stability

$$Q_h y \in R(Q_h A P_h) \qquad \|Q_h A u_h\|_Y \geq \gamma \|u_h\|_X$$

$$+$$

$$P_h u \to u \ \ \& \ \ Q_h y \to y \qquad \|Q_h A u - Q_h A P_h u\|_Y \to 0$$

approximation

Variational compatibility

$$\Downarrow$$

Unique solvability and quasi-optimal convergence

$$\|u - u_h\|_X \leq \|P_h u - u\|_X + \frac{1}{\gamma}\|Q_h A u - Q_h A P_h u\|_Y$$

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Variational settings for FEM

Optimization | **No optimization**

$$\underbrace{\min_{v\in X}\frac{1}{2}\langle Av,v\rangle-\langle f,v\rangle \qquad \min_{v\in X}\frac{1}{2}\langle Av,v\rangle-\langle f,v\rangle \text{ subject to } Bv=0}_{}$$

$$X\ni u\perp_{\mathcal{K}}Y$$

$$\mathcal{K}(u-u,v)=0\ \ \forall v\in Y$$

seek $u\in X$ s.t. $\mathcal{K}(u,v)=F(v)\quad \forall v\in Y$

FEM = variational principle + piecewise polynomial subspaces

seek $u_h\in X_h$ s.t. $\mathcal{K}(u_h,v_h)=F(v_h)\quad \forall v_h\in Y_h$

$$((u-u_h,v_h))_{\mathcal{K}}=0 \quad \forall v_h\in X_h$$

$$\underbrace{\begin{aligned}&a(u_h,v_h)+b(p_h,v_h)=(f,v_h)\ \forall v_h\in V_h\\&b(q_h,u_h)=0 \qquad \forall q_h\in P_h\end{aligned} \qquad \begin{aligned}&\mathcal{K}(u-u_h,v_h)=0\ \forall v_h\in Y_h\\&X_h\ni u_h\perp_{\mathcal{K}}Y_h\end{aligned}}_{}$$

Projection | **Quasi-projection**

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Examples

No Optimization

- Advection-Diffusion-Reaction models
- Navier-Stokes equations

Constrained Optimization

Kelvin principle:

- the **solenoidal** velocity field that minimizes kinetic energy is **irrotational**

Dirichlet principle:

- the **irrotational** velocity field that minimizes kinetic energy is **solenoidal**

Unconstrained Optimization

- Poisson equation

No Optimization

Variational problem

$$\mathcal{K}(u,v) = F(v) \quad \forall v \in Y$$

$\forall u \in X \quad \exists v \in Y$ s.t.

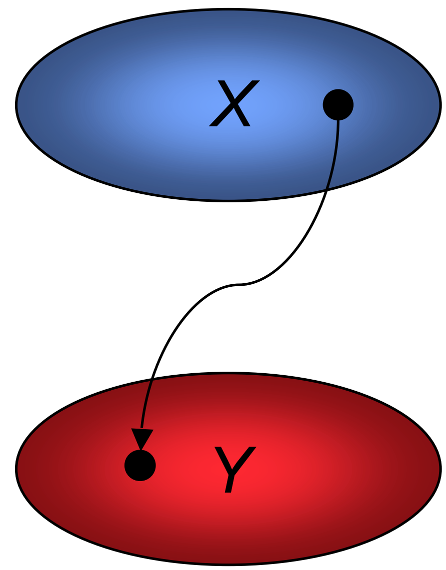
$$\mathcal{K}(u,v) \geq C\|u\|_X \|v\|_Y$$

Unique solvability & stability

$$\mathcal{K}(u,v) \leq \alpha\|u\|_X \|v\|_Y$$ continuity

$$\sup_{v\in Y} \frac{\mathcal{K}(u,v)}{\|v\|_Y} \geq \gamma\|u\|_X \quad \forall u \in X$$ Inf-sup (I)

$$\sup_{u\in X} \frac{\mathcal{K}(u,v)}{\|u\|_X} \geq 0 \qquad \forall v \in Y$$ Inf-sup (II)



$$\boxed{\|u\|_X \leq C\|F\|}$$

Compatibility

Discrete problem

$$\mathcal{K}(u_h, v_h) = F(v_h) \quad \forall v_h \in Y_h \qquad\qquad K_h u_h = F_h$$

Variational compatibility

conformity: $X_h \subset X; \quad Y_h \subset Y \;\Rightarrow$ **continuity**

Necessary but insufficient!

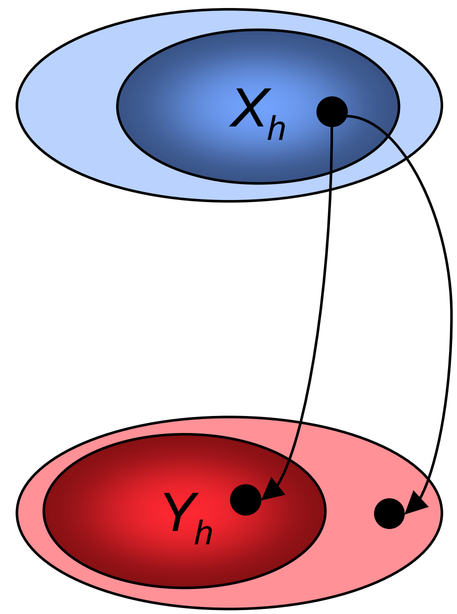
Inf-sup (I) $$\sup_{v_h \in Y_h} \frac{\mathcal{K}(u_h, v_h)}{\|v_h\|_{Y_h}} \geq \gamma_h \|u_h\|_X \quad \forall u_h \in X_h$$

Inf-sup (II) $$\sup_{u_h \in X_h} \frac{\mathcal{K}(u_h, v_h)}{\|u_h\|_{X_h}} \geq 0 \qquad \forall v_h \in Y_h$$

$$\|u_h\|_X \leq C\|F\| \qquad \|u - u_h\|_X \leq \left(1 + \frac{1}{\gamma_h}\right) \inf_{v_h \in X_h} \|u - v_h\|_X$$

$\forall u_h \in X_h \quad \exists v \in Y$ s.t.

$$\mathcal{K}(u_h, v) \geq C\|u_h\|_X \|v\|_Y$$



$\forall u_h \in X_h \quad \exists v_h \in Y_h$ s.t.

$$\mathcal{K}(u_h, v_h) \geq C\|u_h\|_X \|v_h\|_X$$

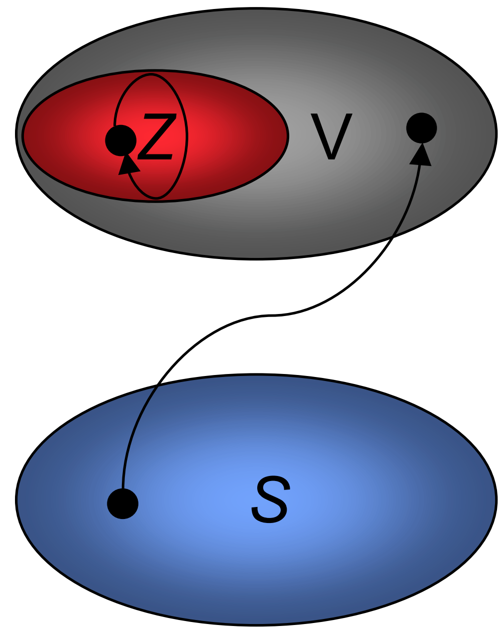
Constrained Optimization

Variational problem $X = Y = V \times S$

$$\min_{v\in V}\max_{q\in S}\frac{1}{2}\langle Av,v\rangle - \langle f,v\rangle - \langle Bv,q\rangle$$

$$\begin{aligned} a(u,v) + b(p,v) &= (f,v) \quad && \forall v \in V \\ b(q,u) &= 0 && \forall q \in S \end{aligned}$$

$$Z = \ker B = \{v \in X \mid Bv = 0\}$$



Unique solvability & stability

continuity of *a* and *b*

$$a(v,v) \ge C_a \|v\|_X \qquad \forall v \in Z$$ **coercivity on *Z***

$$\sup_{v\in V}\frac{b(p,v)}{\|v\|_V} \ge \gamma_b \|p\|_Q \quad \forall p \in S$$ **inf-sup for B**

$$\forall p \in S \quad \exists v \in V \text{ s.t.}$$

$$b(p,v) \ge \gamma \|p\|_S \|v\|_V$$

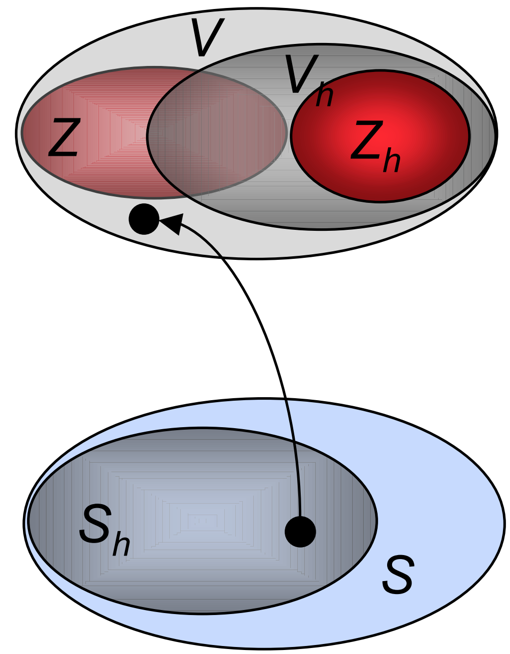
$$\boxed{\|u\|_V + \|p\|_S \le C\|f\|_{V^*}}$$

Compatibility

Discrete Problem

$$Au + B^* p = F \qquad Bu = 0 \quad \Rightarrow \quad \begin{pmatrix} A_h & B_h^T \\ B_h & 0 \end{pmatrix} \begin{pmatrix} v_h \\ p_h \end{pmatrix} = \begin{pmatrix} f_h \\ 0 \end{pmatrix}$$

$$Z_h = \{ v_h \in S_h \mid b(v_h, q_h) = 0 \ \forall q_h \in V_h \} \not\subset Z$$



Variational compatibility

conformity $V_h \subset V; \quad S_h \subset S \Rightarrow$ **continuity**

$$\forall p_h \in S_h \quad \exists v \in V \text{ s.t. } b(p_h, v) \geq \gamma \|p_h\|_S \|v\|_V$$

Necessary but insufficient:

$$\exists v_h \in V_h \text{ s.t. } b(p_h, v_h) \geq \gamma \|p_h\|_S \|v_h\|_V \ ?$$

$$Z_h \neq \varnothing ?$$

$$Z_h \neq \varnothing : \qquad Z_h \not\subset Z \quad \Rightarrow \quad a(v_h, v_h) \geq C_a \|v_h\|_V \quad \forall v_h \in Z_h \ ??$$

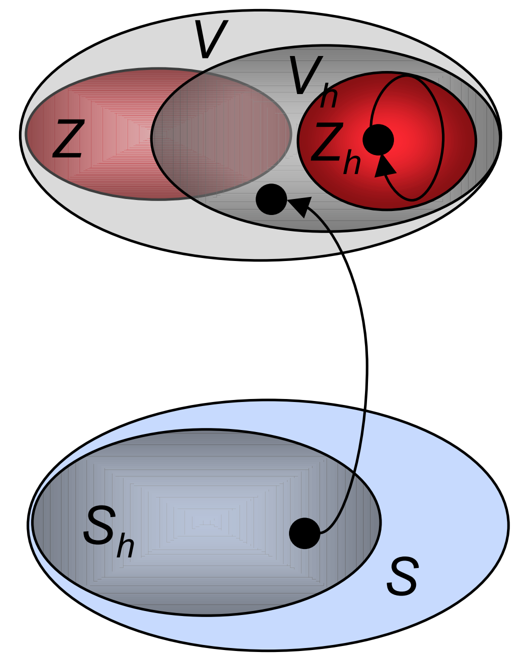
Variational compatibility

conformity $\quad V_h \subset V; \quad S_h \subset S$

coercivity on Z_h $\quad a(v_h, v_h) \geq C_a \|v_h\|_V \quad \forall v_h \in Z_h;$

inf-sup for B_h $\quad \sup\limits_{v_h \in V_h} \dfrac{b(p_h, v_h)}{\|v_h\|_V} \geq \gamma_h \|p_h\|_S \quad \forall p_h \in S_h$

$Z_h \neq \emptyset; \quad \forall p_h \in S_h \quad \exists v_h \in V_h$ s.t. $b(p_h, v_h) \geq \gamma \|p_h\|_S \|v_h\|_V$



$$\|u_h\|_V + \|p_h\|_S \leq C \|f\|_{V^*}$$

$$\|u - u_h\|_V \leq C_1 \inf_{v_h} \|u - v_h\|_V + C_2 \Theta(Z, Z_h) \inf_{q_h} \|p - q_h\|_S$$

$$\|p - p_h\|_S \leq C_3 \inf_{v_h} \|u - v_h\|_V + C_4 \inf_{q_h} \|p - q_h\|_S$$

Unconstrained Optimization

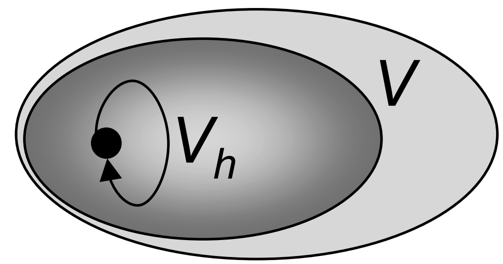
Variational problem $X = Y$

$$\min_{v \in X} \frac{1}{2}\langle Av, v\rangle - \langle f, v\rangle \qquad \mathcal{K}(u,v) = F(v) \quad \forall v \in X$$

Unique solvability & stability

$$\mathcal{K}(u,v) \le C_b \|u\|_X \|v\|_X$$ **continuity**

$$\mathcal{K}(v,v) \ge C_a \|v\|_X^2 \ \forall v \in X$$ **coercivity**



Discrete problem

$$\mathcal{K}(u_h, v_h) = F(v_h) \quad \forall v_h \in Y_h \qquad K_h u_h = F_h$$

$$\mathcal{K}(v_h, v_h) \ge C_a \|v_h\|_X^2 \ \forall v_h \in X_h$$

Variational compatibility

conformity: $X_h \subset X \;\Rightarrow$ **continuity & coercivity!**

$$\|u_h\|_X \le C\|F\| \qquad \|u - u_h\|_X \le \frac{1}{C_a} \inf_{v_h \in X_h} \|u - v_h\|_X$$

A summary of variational settings for FEM

Features	*Variational setting*		
	Optimization type		
	Unconstrained	*constrained*	*None*
Unique solvability	Continuity Coercivity	Continuity Coercivity on Z Inf-sup for B	Continuity Inf-sup (I) Inf-sup (II)
Variational compatibility	Conformity	Conformity Coercivity on Z_h Inf-sup for B_h	Conformity Inf-sup(I) Inf-sup(II)
Algebraic problem type	Symmetric positive definite	Symmetric indefinite	None

What does variational compatibility buy you

Sequence stability is equivalent to variational compatibility

$$\inf_{u_h}\sup_{v_h}\frac{v_h^T K_h u_h}{\|v_h\|_X\|u_h\|_X}\geq\gamma \quad\Leftrightarrow\quad \inf_{u_h}\sup_{v_h}\frac{\mathcal{K}(u_h,v_h)}{\|v_h\|_X\|u_h\|_X}\geq\gamma$$

Allows to assert powerful results about the asymptotic behavior

- quasi-optimal **error estimates**
- unique **solvability** for any *h*
- **stability** of discrete solutions (uniform invertibility)

This answers the 1st question:

1. **Is the family of algebraic equations well-behaved?**
   - are all problems **uniquely** and **stably** **(**in *h***)** solvable?
   - do solutions **converge** to the exact solutions as $h \rightarrow 0$?

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What does variational compatibility say about the other issues?

Not much

Variational compatibility conditions are not constructive!

These conditions are not very helpful in finding the stable spaces and may be difficult to verify. Creative application of non-trivial tricks required, e.g.,

— Fortin's operator

— Verfurth's method

— Boland & Nicolaides's method

Inf-sup fear and loathing still common!

“Pure” Direct Discretizations

Algebraic model

Kinematic relation

$$u_1 = p_2 - p_1$$
$$u_2 = p_3 - p_2$$
$$u_3 = p_4 - p_1$$
$$u_4 = p_5 - p_2$$
$$u_5 = p_6 - p_3$$
$$u_6 = p_5 - p_4$$
$$u_7 = p_6 - p_5$$
$$u_8 = p_7 - p_4$$
$$u_9 = p_8 - p_5$$
$$u_{10} = p_9 - p_6$$
$$u_{11} = p_8 - p_7$$
$$u_{12} = p_9 - p_8$$

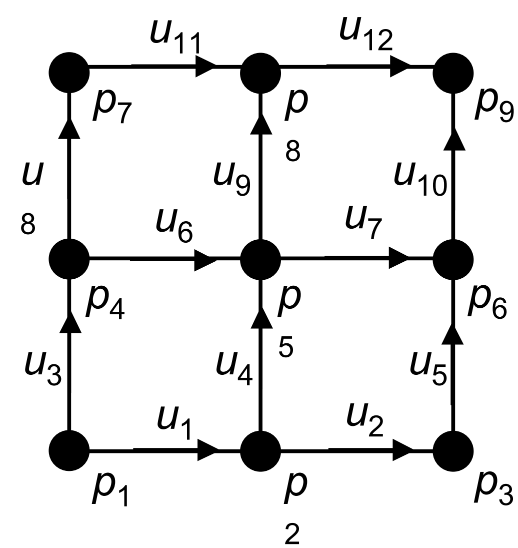
Constitutive equation

$$v_i = \rho_i u_i$$

Continuity relation

$$-v_1 - v_3 = 0$$
$$+v_1 - v_2 - v_4 = 0$$
$$+v_2 - v_5 = 0$$
$$+v_3 - v_6 - v_8 = 0$$
$$+v_4 + v_6 - v_7 - v_9 = 0$$
$$+v_7 + v_5 - v_{10} = 0$$
$$+v_8 - v_{11} = 0$$
$$+v_9 + v_{11} - v_{12} = 0$$
$$+v_{10} + v_{12} = 0$$

Reduced system



$p \rightarrow$ "pressure"

$u \rightarrow$ "velocity"

$\rho \rightarrow$ "density"

$v \rightarrow$ "flow"

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The Hodge

A possible “physical” interpretation of Hodge:
(Franco’s question)

Conversion of velocity (measured along a line)
into a flow (measured across a surface)

Problems with identical reduced systems

	Potential flow	***Thermal diffusion***	***Electro statics***	***Linear elasticity***	***Electrical network***
p	Pressure	Temperature	Potential	Displacement	Potential
u	Velocity	Heat flux	Electric field	Strain	Voltage
A^{-1}	Permeability	Thermal conductivity	Conductivity Ohm's law	Compliance Hook's law	Conductivity Ohm's law
v	Flow rate	Heat flow	Current	Stress	Current
f	Fluid Source	Heat Source	Source Current	Applied load	Applied current
g	N/A	Heat battery	Battery	N/A	Battery

Matrix Form

Kinematic	Constitutive	Continuity
$u + B^T p = g$	$u = Av$	$Bu = f$

$$\begin{pmatrix}
-1 & 1 & & & & & & & \\
 & -1 & 1 & & & & & & \\
-1 & & & 1 & & & & & \\
 & -1 & & & 1 & & & & \\
 & & -1 & & & 1 & & & \\
 & & & -1 & 1 & & & & \\
 & & & & -1 & 1 & & & \\
 & & & -1 & & & 1 & & \\
 & & & & -1 & & & 1 & \\
 & & & & & -1 & & & 1 \\
 & & & & & & -1 & 1 & \\
 & & & & & & & -1 & 1
\end{pmatrix}
\qquad
\begin{pmatrix}
\frac{1}{\rho_i} & & \\
 & \ddots & \\
 & & \frac{1}{\rho_i}
\end{pmatrix}
\qquad
\begin{pmatrix}
-1 & & -1 & & & & & & & & & \\
1 & -1 & & -1 & & & & & & & & \\
 & 1 & & & -1 & & & & & & & \\
 & & 1 & & & -1 & & -1 & & & & \\
 & & & 1 & & 1 & -1 & & -1 & & & \\
 & & & & 1 & & 1 & & & -1 & & \\
 & & & & & & & 1 & & & -1 & \\
 & & & & & & & & 1 & & 1 & -1 \\
 & & & & & & & & & 1 & & 1
\end{pmatrix}$$

Note that if we were to **build** the reduced system, its behavior will be described **exactly** by this algebraic equation!

$$\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}\begin{pmatrix} v \\ p \end{pmatrix} = \begin{pmatrix} g \\ f \end{pmatrix}$$

$$-BA^{-1}B^T p = f - BA^{-1}g$$

Geometric compatibility

Geometrically compatible discretization:

algebraic equations that describe "actual" physical systems.

Requires to discover structure and invariants of physical systems and then copy them to a discrete system

- Fields are observed **indirectly** by measuring **global** quantities (flux, circulation, etc)
- Physical laws are **relationships** between **global** quantities (conservation, equilibrium)

Differential forms provide the tools to encode such relationships

- **Integration:** an abstraction of the *measurement* process
- **Differentiation:** gives rise to *local invariants*
- **Poincare Lemma:** expresses *local geometric* relations
- **Stokes Theorem:** expresses *global relations* (differentiation + integration)

How to achieve geometric compatibility?

Algebraic topology provides the tools to copy the structure

1. System states are **differential forms** reduced to **co-chains**
2. Exterior **differentiation** approximated by the **co-boundary** operator
3. **Dual** operators defined using **Hodge *** operator

Branin (1966), Dodzuik (1976), Hyman & Scovel (1988-92), Mattiussi (1997), Teixeira (2001)

Mimetic and co-volume methods fit this reduction model

- **Vector fields** represented by their integrals (fluxes or circulations)
- **Differential operators** defined via Stokes Theorem (coordinate-invariant)
- **Primal and dual** equations/operators (B and B^T) and an inner product (A)

Algebraic Topology Approach
1. System reduction

3 exact sequences: $(W_0, W_1, W_2, W_3), (C_0, C_1, C_2, C_3), (C^0, C^1, C^2, C^3)$

forms $\cdots W_k \xrightarrow{d} W_{k+1} \cdots$

$\downarrow \qquad \downarrow \quad \leftarrow \quad \mathcal{R} : W_k \to C^k, \quad \langle \mathcal{R}\omega, c \rangle = \int_c \omega$

co-chains $\cdots C^k \xrightarrow{\delta} C^{k+1} \cdots$

DeRham map

$\updownarrow \qquad \updownarrow$

chains $\cdots C_k \xrightarrow{\partial} C_{k+1} \cdots$

Fundamental property: $\mathcal{R}d = \delta\mathcal{R}$

$$\langle \delta\mathcal{R}\omega, c \rangle = \langle \mathcal{R}\omega, \partial c \rangle = \int_{\partial c} \omega = \int_c d\omega = \langle \mathcal{R}d\omega, c \rangle$$

Commuting Diagram I

$$\begin{tikzcd} W_k \arrow[r, "d"] \arrow[d, "\mathcal{R}"'] & W_{k+1} \arrow[d, "\mathcal{R}"] \\ C^k \arrow[r, "\delta"] & C^{k+1} \end{tikzcd}$$

$\{G,D,C\} \leftarrow \delta$ approximates $d \rightarrow \{\text{grad,curl,div}\}$

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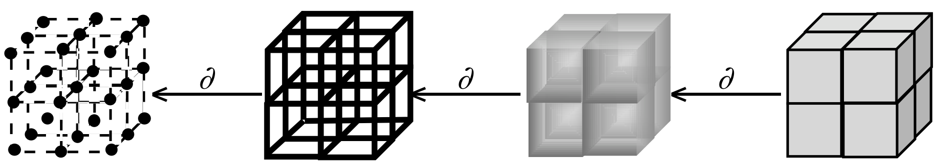
Example

chains

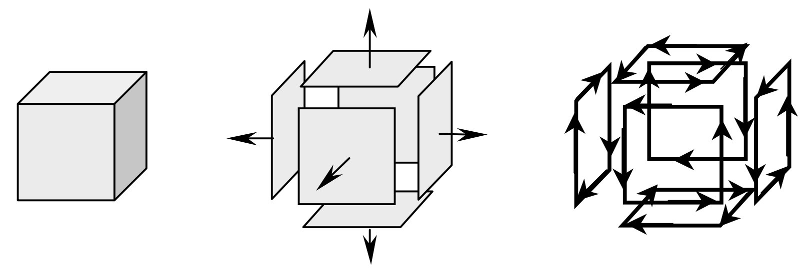


$$\int_c \omega$$

$$N \xrightarrow{\delta} E \xrightarrow{\delta} F \xrightarrow{\delta} K$$

co-chains

$\partial\partial = 0$



$$K \xrightarrow{\partial} \partial K \xrightarrow{\partial} \partial\partial\, K = 0$$

$$\left\langle \delta c^k, c_{k+1} \right\rangle = \left\langle c^k, \partial c_{k+1} \right\rangle$$

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 1 & 1 & -1 & -1 & 1 \end{pmatrix}$$

$\delta\delta = 0$

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Algebraic Topology Approach
2. Inner products and dual operators

Inner product $W_k \times W_k$

$$* : W_k \to W_{n-k} \qquad (\omega,\varphi)_W = \int_\Omega \omega \wedge *\varphi$$

Inner product $C^k \times C^k$

$$\mathcal{I} : C^k \to W_k \qquad (a,b)_c = (\mathcal{I}a,\mathcal{I}b) = \int_\Omega \mathcal{I}a \wedge *\mathcal{I}b = \mathbf{a}^T\mathbf{Mb}$$

Dual operators

$$(\delta a,b)_c = (a,\delta^* b) \quad \to \quad \boldsymbol{G^*, C^*, D^*}$$

C*G*=D*C*=0 **requires** $d\mathcal{I} = \mathcal{I}\delta$

Commuting Diagram II

$$\begin{tikzcd} C^k \arrow[r, "\delta"] \arrow[d, "\mathcal{I}"'] & C^{k+1} \arrow[d, "\mathcal{I}"] \\ W_k \arrow[r, "d"] & W_{k+1} \end{tikzcd}$$

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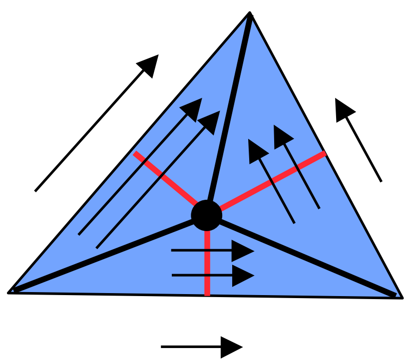
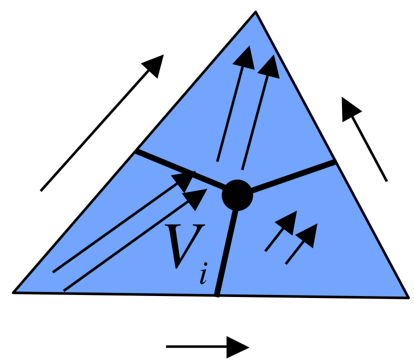
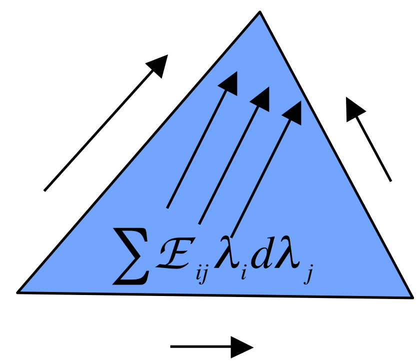
Examples

	Co-volume	Mimetic	Whitney
$\mathcal{J}$			
	Nicolaides, Trapp (1992-04)	*Hyman, Shashkov, Steinberg (1985-04)*	*Dodzuik (1976) Hyman, Scovel (1988)*
M	$\begin{pmatrix} h_1 h_1^{\perp} & & \\ & h_2 h_{21}^{\perp} & \\ & & h_3 h_3^{\perp} \end{pmatrix}$	$\begin{pmatrix} \frac{V_2}{\sin^2\phi_2}+\frac{V_3}{\sin^2\phi_3} & \frac{V_3\cos\phi_3}{\sin^2\phi_3} & \frac{V_2\cos\phi_2}{\sin^2\phi_2} \\ \frac{V_3\cos\phi_3}{\sin^2\phi_3} & \frac{V_1}{\sin^2\phi_1}+\frac{V_3}{\sin^2\phi_3} & \frac{V_1\cos\phi_1}{\sin^2\phi_1} \\ \frac{V_2\cos\phi_2}{\sin^2\phi_2} & \frac{V_1\cos\phi_1}{\sin^2\phi_1} & \frac{V_1}{\sin^2\phi_1}+\frac{V_2}{\sin^2\phi_2} \end{pmatrix}$	$\begin{pmatrix} \cdots & \cdots & \cdots \\ \cdots & (w_{ij}, w_{kl}) & \\ \cdots & \cdots & \cdots \end{pmatrix}$

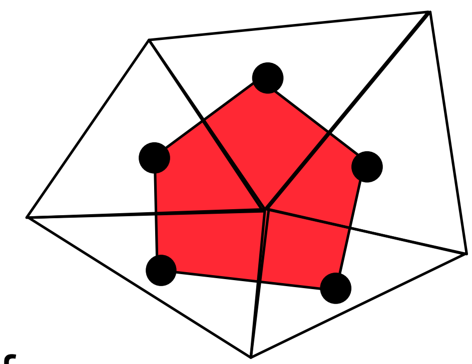
Properties

Co-volume inner product is the unique inner product that is

- ✓ **diagonal**
- ✓ **exact** for constant vector fields

⇒ Important computational property:

- ✓ dual co-volume operators have **local** stencils



Stencil of *D**

Action of co-volume and mimetic products coincides if

$$V_i = |\mathbf{t}| \frac{\tan \phi_i}{\sum \tan \phi_k}$$ *(Trapp, 2004)*

Approximation

$$\mathcal{I}_{\text{Mim/co}}(\mathcal{R}\omega) - \omega = O(h^2)/O(h)$$ *(Shashkov, Wheeler, Yotov 2004/ Trapp, 2004)*

$$\mathcal{I}_{\text{Whitney}}(\mathcal{R}\omega) - \omega = O(h)$$ *(Dodzuik, 1976)*

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Algebraic Topology Framework: Summary

1. **Structures:**

   (W_0, W_1, W_2, W_3) Forms

   (C_0, C_1, C_2, C_3) Chains

   (C^0, C^1, C^2, C^3) Co-chains

2. **De Rham map**

   $\mathcal{R} : W_k \to C^k$ $\quad\quad$ $\mathcal{R}d = \delta\mathcal{R}$

3. **Interpolation operator**

   $\mathcal{I} : C^k \to W_k$ $\quad\quad$ $d\mathcal{I} = \mathcal{I}\delta$

4. **Inner product**

   $(a,b)_c = (\mathcal{I}a, \mathcal{I}b)$ $\quad\quad$ $\mathbf{M}$

5. **Primal and dual operators**

   $\{G,C,D\}$ & $\{G^*,C^*,D^*\}$

Geometric compatibility

$$\begin{tikzcd} W_k \arrow[r, "d"] \arrow[d, "\mathcal{R}"'] & W_{k+1} \arrow[d, "\mathcal{R}"] \\ C^k \arrow[r, "\delta"] & C^{k+1} \end{tikzcd}$$

CDP 1

$$\begin{tikzcd} C^k \arrow[r, "\delta"] \arrow[d, "\mathcal{I}"'] & C^{k+1} \arrow[d, "\mathcal{I}"] \\ W_k \arrow[r, "d"] & W_{k+1} \end{tikzcd}$$

CDP 2

Direct discretization of a div-curl system

$$\mathbf{n}\times\mathbf{u}=h \quad \text{on } \Gamma \qquad \begin{array}{l} \nabla\times\mathbf{u}=\mathbf{f} \quad \text{in } \Omega \\ \nabla\cdot\mathbf{u}=g \quad \text{in } \Omega \end{array} \qquad \text{on } \Gamma \quad h=\mathbf{n}\cdot\mathbf{u}$$

$$\mathbf{u}\in C^1 \rightarrow \left\{ \begin{array}{l} C: C^1 \rightarrow C^2 \\ D^*: C^1 \rightarrow C^0 \end{array} \right. \qquad \begin{array}{l} \nabla\times \rightarrow d_1 \\ \nabla\cdot \rightarrow d_2 \end{array} \qquad \left. \begin{array}{l} C^*: C^2 \rightarrow C^1 \\ D: C^2 \rightarrow C^3 \end{array} \right\} \leftarrow \mathbf{u}\in C^2$$

$$\mathbf{u}=h \quad \text{on } C^1/C^1_\Gamma \qquad \begin{array}{l} C\mathbf{u}=\mathbf{f} \quad \text{in } C^2 \\ D^*\mathbf{u}=g \quad \text{in } C^0 \end{array} \qquad \begin{array}{l} C^*\mathbf{u}=\mathbf{f} \quad \text{in } C^1 \\ D\mathbf{u}=g \quad \text{in } C^3 \end{array} \qquad \mathbf{u}=h \quad \text{on } C^2/C^2_\Gamma$$

Examples:

Co-volume: *Nicolaides et. al. 1992-2004*

Finite difference: *Yee, 1966*

Finite volume: *Weiland, 1977*

Direct discretization of a div-grad system

$$\mathbf{n}\cdot\mathbf{u}=h \quad \text{on } \Gamma \qquad \begin{array}{ll} \nabla\cdot\mathbf{u}=\mathbf{f} & \text{in } \Omega \\ \nabla\varphi+\mathbf{u}=0 & \text{in } \Omega \end{array} \qquad \text{on } \Gamma \quad h=\varphi$$

$$\left.\begin{array}{l}\mathbf{u}\in C^2\\ \varphi\in C^3\end{array}\right\}\rightarrow\left\{\begin{array}{l}D:C^2\rightarrow C^3\\ G^*:C^3\rightarrow C^2\end{array}\right. \qquad \begin{array}{l}\nabla\cdot\rightarrow d_2\\ \nabla\rightarrow d_0\end{array} \qquad \left.\begin{array}{r}D^*:C^1\rightarrow C^2\\ G:C^0\rightarrow C^1\end{array}\right\}\leftarrow\left\{\begin{array}{l}\mathbf{u}\in C^1\\ \varphi\in C^0\end{array}\right.$$

$$\mathbf{u}=h \quad \text{on } C^2/C^2_\Gamma \qquad \begin{array}{ll} D\mathbf{u}=f & \text{in } C^3 \\ G^*\varphi+\mathbf{u}=0 & \text{in } C^2 \end{array} \qquad \begin{array}{ll} D^*\mathbf{u}=f & \text{in } C^2 \\ G\varphi+\mathbf{u}=0 & \text{in } C^1 \end{array} \qquad \varphi=h \quad \text{on } C^0/C^0_\Gamma$$

Eliminations $\quad -DG^*\varphi=f \qquad -D^*G\varphi=f$

$$-BA^{-1}B^T$$

Examples

Mimetic: *Shashkov et. al. 1995-2004*

Finite volume: The box integration method: *Mock, 1983*

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What does geometric compatibility buy you?

Co-cycles of (W_0, W_1, W_2, W_3) $\xrightarrow{\mathcal{R}}$ co-cycles of (C^0, C^1, C^2, C^3)

$$d\omega = 0 \quad \Rightarrow \quad \delta \mathcal{R}\omega = 0$$

Discrete Poincare lemma (existence of potentials in contractible domains)

$$d\omega_k = 0 \quad \Rightarrow \quad \omega_k = d\omega_{k+1} \qquad\qquad \delta c^k = 0 \quad \Rightarrow \quad c^k = \delta c^{k+1}$$

Discrete Stokes Theorem

$$\langle d\omega_{k-1}, c_k \rangle = \langle \omega_{k-1}, \partial c_k \rangle \qquad\qquad \langle \delta c^{k-1}, c_k \rangle = \langle c^{k-1}, \partial c_k \rangle$$

Discrete "Vector Calculus"

$$dd = 0 \qquad\qquad \delta\delta = 0 \rightarrow \quad CG = DC = 0;\ C^*G^* = D^*C^* = 0$$

Any feature of the continuum system that is implied by differential forms calculus is inherited by the discrete model

Called ***mimetic*** property by Hyman and Scovel (1988)

Solvability: free of charge

Div-curl system: Discrete Helmholtz orthogonality

$$\left.\begin{array}{l} C\mathbf{u}=0 \\ D^{*}\mathbf{v}=0 \end{array}\right\} \Rightarrow (\mathbf{u},\mathbf{v})_{C^1}=0 \qquad \left.\begin{array}{l} C\mathbf{u}=0 \\ D^{*}\mathbf{u}=0 \end{array}\right\} \Rightarrow (\mathbf{u},\mathbf{u})_{C^1}=0 \Rightarrow \mathbf{u}\equiv 0$$

Div-grad system: Commuting diagram property

Unique solvability: $G^{*}\varphi=0 \Rightarrow \varphi=0$

Assume: $\varphi \in C^{3}; G^{*}\varphi=0$ but $\varphi \neq 0$

CDP I

$$\begin{array}{ccc} W_2 & \xrightarrow{d} & W_3 \\ \mathcal{R}\downarrow & & \downarrow\mathcal{R} \\ C^2 & \xrightarrow{\delta} & C^3 \end{array}$$

surjection

surjection $\quad \forall\varphi \in C^{3} \quad \exists\mathbf{u}_{\varphi} \in C^{2}$ s.t. $\varphi = D\mathbf{u}_{\varphi}$

$0=(\mathbf{u}_{\varphi},G^{*}\varphi)=(D\mathbf{u}_{\varphi},\varphi)=(\varphi,\varphi)\neq 0$, a contradiction!

Variational vs. geometric

Variational

- **Operator**-centric point of view
  - **Problem** = operator equation on function spaces
  - **Discretization** = operator equation + functional approximation
- Stability conditions
- Error estimates

stability conditions not constructive -
do not reveal structure of stable discretizations

Geometric

- **Topology**-centric point of view
  - **Problem** = equilibrium relation on manifolds
  - **Discretization** = equilibrium relation + manifold approximation
- Forces **physically compatible** discretization patterns
- Preserves problem structure

Variational and geometric

We can benefit from combining both approaches

D. Arnold — stable mixed spaces designed by association of the problem with a differential complex

M. Shashkov — error analysis of mimetic schemes enabled by identification with a mixed Galerkin method and a proper quadrature selection.

I will now examine **connections** between **geometrical** and **variational** compatibility that validate such collaborations using **Kelvin's principle** as a prototype problem

$$\int_\Omega \psi \nabla \cdot \mathbf{v} d\Omega = \int_\Omega \psi f \, d\Omega \quad \forall \psi \in S$$
$$\int_\Omega \mathbf{v} \cdot \mathbf{w} - \varphi \nabla \cdot \mathbf{w} d\Omega = 0 \quad \forall \mathbf{w} \in V$$

$$\min_{v \in V} \max_{q \in S} \frac{1}{2} \int_\Omega |\mathbf{v}|^2 d\Omega - \int_\Omega \varphi (\nabla \cdot \mathbf{v} - f) d\Omega$$

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Early examples

Grid Decomposition Property

$$\mathbf{v} \in \mathbf{L}^2 \qquad \left.\begin{array}{l} \mathbf{v} = \mathbf{w} + \mathbf{z} \\ \nabla \cdot \mathbf{z} = 0 \end{array}\right\} \quad \text{geometry} \quad \left\{\begin{array}{l} \mathbf{v}^h = \mathbf{w}^h + \mathbf{z}^h \\ \nabla \cdot \mathbf{z}^h = 0 \end{array}\right. \qquad \mathbf{v}^h \in V^h$$

Helmholtz **GDP**

$$(\mathbf{w},\mathbf{z}) = 0\Big\} \quad \text{metric} \quad \left\{\begin{array}{l} (\mathbf{w}^h,\mathbf{z}^h) = 0 \\ \|\mathbf{w}^h\|_0 \le C\left(\|\nabla \cdot \mathbf{v}^h\|_{-1} + \|\nabla \cdot \mathbf{v}^h\|_0\right) \end{array}\right.$$

Theorem

GDP is *necessary* and *sufficient* for stable, optimally accurate mixed discretization of the Kelvin principle.

Fix, Gunzburger, Nicolaides, ICASE Report 78-7, 1977, Num. Math, 1981

Similar GDP exists for the Dirichlet principle but is trivial to satisfy!

Early examples

Fortin Lemma

(V^h, S^h) verify inf-sup condition for the Kelvin principle iff:

$$\Pi_h : V \to V^h \begin{cases} \int_\Omega \nabla \cdot (\Pi_h \mathbf{v}) \psi_h \, d\Omega = \int_\Omega \nabla \cdot \mathbf{v} \psi_h \, d\Omega & \text{geometry} \\ \|\Pi_h \mathbf{v}\|_V \le C \|\mathbf{v}\|_V & \text{metric} \end{cases}$$

Geometric assumption:

$$\int_\Omega \psi_h \nabla \cdot (\Pi_h \mathbf{v}) d\Omega = \int_\Omega \psi_h \nabla \cdot \mathbf{v} d\Omega$$

$$\nabla \cdot (\mathcal{I}_2) = \mathcal{I}_3(\nabla \cdot)$$

equivalent to a *commuting diagram*!

$$\begin{tikzcd} V \arrow[r, "\nabla \cdot"] \arrow[d, "\mathcal{I}_2"'] & S \arrow[d, "\mathcal{I}_3"] \\ V^h \arrow[r, "\nabla \cdot"] & S^h \end{tikzcd}$$

Douglas and Roberts, Math. Appl. Comp. 1982

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Can this be an accident?

We see :

- conditions that combine *geometric* and *metric* properties
- the ubiquitous *commuting diagram*…

The French Connection

Bossavit, Nedelec, Verite, 1982-88 and *Kotiuga, 1984*, were first from the finite element community to notice and document an uncanny connection between unusual, i.e., *not nodal*, finite element spaces and *Whitney forms*.

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Elsewhere…

FINITE-DIFFERENCE APPROACH TO THE
HODGE THEORY OF HARMONIC FORMS.*

By JOZEF DODZIUK.

Table of Contents

G. Strang informed us that the techniques used in this paper are very closely related to finite element method of solving partial differential equations numerically.

CDP 1 + CDP 2 = VC

Geometric compatibility

CDP 1

$$\begin{array}{ccc} W_k & \xrightarrow{d} & W_{k+1} \\ \mathcal{R}\downarrow & & \downarrow\mathcal{R} \\ C^k & \xrightarrow{\delta} & C^{k+1} \end{array}$$

CDP 2

$$\begin{array}{ccc} C^k & \xrightarrow{\delta} & C^{k+1} \\ \mathcal{I}\downarrow & & \downarrow\mathcal{I} \\ W_k & \xrightarrow{d} & W_{k+1} \end{array}$$

Variational compatibility

$$\begin{array}{cccl} W_k & \xrightarrow{d} & W_{k+1} & \quad \textbf{Forms} \\ \mathcal{R}\downarrow & & \downarrow\mathcal{R} & \\ C^k & \xrightarrow{\delta} & C^{k+1} & \quad \textbf{DOFs} \\ \mathcal{I}\downarrow & & \downarrow\mathcal{I} & \\ W_k^h & \xrightarrow{d} & W_{k+1}^h & \quad \textbf{FEMs} \end{array}$$

$$(\mathcal{I}\circ\mathcal{R})\circ d = d\circ(\mathcal{I}\circ\mathcal{R})$$ **CDP**

CDP is equivalent to stability of mixed FEM

CDP and **GDP** are also equivalent!

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There's only one low-order compatible method

Well, up to a choice of an inner product…

And a quadrature rule…

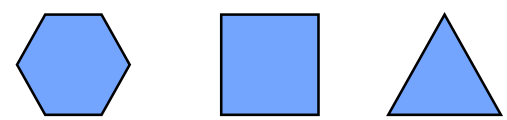
And a cell shape…

$$\begin{tikzcd} W_k \arrow[r, "d"] \arrow[d, "\mathcal{R}"'] & W_{k+1} \arrow[d, "\mathcal{R}"] \\ C^k \arrow[r, "\delta"] \arrow[d, "\mathcal{I}"'] & C^{k+1} \arrow[d, "\mathcal{I}"] \\ W_k^h \arrow[r, "d"] & W_{k+1}^h \end{tikzcd}$$

Co-volume

Mimetic

FEM



Whitney,	1957	simplex
Nedelec,	1980-85	cube, prism
Van Welij,	1985	hexahedron
BD(F)M,	80^s -90^s	many shapes

FEM shapes restricted to those that have a "reference element"!

There are more high-order methods

But they are mostly FEM….Why?

Direct methods:

reliance on the De Rham map limits DOFs to co-chains: *stencils expand*!

Variational methods:

order = **degree** of complete polynomials contained in the space (*Bramble-Hilbert*)

Allows to automate formulation of high-order spaces:

- Define reference space containing desired polynomials
- Glue together into piecewise polynomial space
- Coordinate interpolation and DOFs to provide CDP

$$\Pi d = d\Pi$$

$$\begin{tikzcd}
W_k \arrow[r, "d"] \arrow[dddd, bend right, "\Pi"'] & W_{k+1} \arrow[dddd, bend left, "\Pi"] \\
\vdots & \vdots \\
C^k \arrow[r, "\delta"] & C^{k+1} \\
\vdots & \vdots \\
W_k^h \arrow[r, "d"] & W_{k+1}^h
\end{tikzcd}$$

Demkowicz et. al. TICAM Report (1999), Hiptmair's talk, PIERS 32 (2001), Arnold & Winther Numer. Math. (2002), Winther's talk

Conclusions

Variational:

Stronger in metric-dependent aspects :

- assessment of the asymptotic behavior (error, stability)
- formulation of higher-order methods

Weaker in structure-dependent aspects:

- compatibility conditions not constructive, difficult to verify
- FEM restricted to special cell shapes

Geometric:

Weaker in metric-dependent aspects :

- uniform stability of systems, errors, harder to prove
- higher-order methods not easy to define directly

Stronger in structure-dependent aspects:

- structure of the problem copied automatically
- local/global relationships and invariants preserved
- admit a wider set of cell shapes

Conclusions

Variational + Geometric is better

Enjoy the workshop!

Another viewpoint

Recall the discrete network of pipes…

Constitutive

Kinematic

Continuity

$$
\begin{aligned}
u_1 &= p_2 - p_1 \\
u_2 &= p_3 - p_2 \\
u_3 &= p_4 - p_1 \\
u_4 &= p_5 - p_2 \\
u_5 &= p_6 - p_3 \\
u_6 &= p_5 - p_4 \\
u_7 &= p_6 - p_5 \\
u_8 &= p_7 - p_4 \\
u_9 &= p_8 - p_5 \\
u_{10} &= p_9 - p_6 \\
u_{11} &= p_8 - p_7 \\
u_{12} &= p_9 - p_8
\end{aligned}
$$

$$v_i = \rho_i u_i$$

$$
\begin{aligned}
-v_1 - v_3 &= 0 \\
+v_1 - v_2 - v_4 &= 0 \\
+v_2 - v_5 &= 0 \\
+v_3 - v_6 - v_8 &= 0 \\
+v_4 + v_6 - v_7 - v_9 &= 0 \\
+v_7 + v_5 - v_{10} &= 0 \\
+v_8 - v_{11} &= 0 \\
+v_9 + v_{11} - v_{12} &= 0 \\
+v_{10} + v_{12} &= 0
\end{aligned}
$$

- Kinematic and continuity relations depend only on "network topology" (**incidence matrices**!)
- **Metric** is introduced by the constitutive equation.

This distinct pattern appears over and over in physical models (Tonti, 1974).

It can be used to provide an additional insight into compatible discretizations

Factorization (Tonti) diagrams

De Rham complex

Primal

$$\begin{tikzcd}
W^0 \arrow[r, "\nabla", "d"'] \arrow[d, leftrightarrow] & W^1 \arrow[r, "\nabla\times", "d"'] \arrow[d, leftrightarrow] & W^2 \arrow[r, "\nabla\cdot", "d"'] \arrow[d, leftrightarrow] & W^3 \arrow[d, leftrightarrow] \\
\tilde{W}^3 & \tilde{W}^2 \arrow[l, "\nabla\cdot"', "d"] & \tilde{W}^1 \arrow[l, "\nabla\times"', "d"] & \tilde{W}^0 \arrow[l, "\nabla"', "d"]
\end{tikzcd}$$

Hodge $*$

Dual

"All" 2nd order PDE's

K=1

$$\nabla a = -b \qquad \nabla \cdot \beta = -\alpha$$

$$\alpha = *_\mu a \qquad \beta = *_\varepsilon b$$

$$-\nabla \cdot \varepsilon \nabla a + \mu a = f$$

Discrete De Rham complex

Primal

$$\begin{tikzcd}
W_h^0 \arrow[r, "\nabla", "d_h"'] \arrow[d, leftrightarrow] & W_h^1 \arrow[r, "\nabla\times", "d_h"'] \arrow[d, leftrightarrow] & W_h^2 \arrow[r, "\nabla\cdot", "d_h"'] \arrow[d, leftrightarrow] & W_h^3 \arrow[d, leftrightarrow] \\
\tilde{W}_h^3 & \tilde{W}_h^2 \arrow[l, "\nabla\cdot"', "d_h"] & \tilde{W}_h^1 \arrow[l, "\nabla\times"', "d_h"] & \tilde{W}_h^0 \arrow[l, "\nabla"', "d_h"]
\end{tikzcd}$$

Hodge $*_h$

Dual

Tonti (1974), PIERS 32 (2001), Bossavit IEEE Mag. (1988), Hiptmair Num. Math. (2001)

Elimination "**All**" Methods *Primal-dual*

- *One DDF set used*
- *One set eliminated*
- *One **d** is exact*
- *One **d** is weak*
- *One grid only*
- ***Typical:***

  Mixed FEM

  Mimetic FD

- *Two DDF sets used*
- *Two **d**'s are **exact***
- *Two grids (**P**&**D**)*
- ***Typical:***

  Co-Volume

  Staggered grid